# Calculation of the Polarizability and Dipole Moments of Halocarbons in the Liquid State

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Recent measurements of the dielectric permitivity of hydrofluorocarbons in the liquid sate allowed the calculation of the dipole moments in the liquid environment. These values were extracted from Kirkwood theory, and shown to be greater than the dipole moments of the same molecules in the gas phase (isolated molecules).

In order to understand some special features found suggesting possible hindered rotation of some of the molecules, theoretical calculations have been performed.

Density functional and density functional self-consistent reaction field calculations for a series of HFC molecules including $CH_2FCF_3$ (HFC-134a), $CHF_2CH_3$ (HFC-152a), $CHF_2CF_3$ (HFC-125), and $CH_3CF_3$ (HFC-143a), are reported. A particular emphasis has been given to the calculation of electronic polarizabilities and to the prediction of the dipole moment in a dielectric medium representing the liquid environment. The liquid was assumed with no structure and with a constant dielectric constant. Optimised structures for dimers of HFC molecules are also reported.

Our main conclusion is that the present approach, based on the SCIPCM model, underestimates the dipole moment in the liquid phase.